Available online at www.sciencedirect.com

ScienceDirect

J. Math. Anal. Appl. 338 (2008) 840–851

Journal of MATHEMATICAL ANALYSIS AND APPLICATIONS

www.elsevier.com/locate/jmaa

Determining dimension of the solution component that contains a computed zero of a polynomial system

Y.C. Kuo [a], T.Y. Li [b,*,1]

[a] *Department of Applied Mathematics, National University of Kaohsiung, Kaohsiung 811, Taiwan*
[b] *Department of Mathematics, Michigan State University, E. Lansing, MI 48824, USA*

Received 13 May 2006

Available online 2 June 2007

Submitted by W.L. Wendland

Abstract

When the Jacobian of a computed numerical solution of a polynomial system in $\mathbb{C}^n$ allows very small singular values, the solution could be isolated with a multiple multiplicity or may belong to a solution component with positive dimension. The algorithm constructed in this article intends to differentiate those cases by determining the dimension of the solution component $\mathcal{M}$ in which the solution lies. Of particular interest is the case when $\dim(\mathcal{M}) = 0$, then the solution is of course isolated. While the proposed algorithm is experimental, it has been tested successfully on the class of problems with the solution in question belonging to a reduced component. Numerical results are provided to illustrate the accuracy of the algorithm.

Keywords: Homotopy continuation method; Polynomial systems; Solution component

1. Introduction

Let $P(x) = (p_1(x), \ldots, p_n(x))$ be a system of n polynomial equations in the n unknowns $x = (x_1, \ldots, x_n)$ in $\mathbb{C}^n$. When a numerical solution x_0 of $P(x) = 0$ is obtained, by the homotopy continuation method [3–5,15] for instance, x_0 distinguishes itself as an isolated nonsingular solution of $P(x) = 0$ when none of the singular values of the Jacobian of $P(x)$, denoted by $P_X(x)$, at x_0 are too *small*. When $P_X(x_0)$ allows very small singular values, x_0 may lie in a solution component of $P(x) = 0$ with positive dimension or it may still be an isolated solution with multiplicity $\geqslant 2$. The main purpose of this paper is the presentation of an algorithm to differentiate those cases by determining the dimension of the solution component $\mathcal{M}$ of $P(x) = 0$ in which x_0 lies. Of particular interest is the case when $\dim(\mathcal{M}) = 0$, then x_0 is of course an isolated solution of $P(x) = 0$.

The main strategy of our algorithm can be briefly described as follows. If the Jacobian $P_X(x_0)$ has no small singular values, x_0 can be identified as an isolated nonsingular solution. If $P_X(x_0)$ permits only one singular value that appears very small and x_0 is not geometrically isolated, then x_0 must lie in a one-dimensional solution path of $P(x) = 0$.

* Corresponding author.
E-mail address: li@math.msu.edu (T.Y. Li).
[1] Research supported in part by NSF under Grant DMS-0411165.

0022-247X/$ – see front matter
doi:10.1016/j.jmaa.2007.05.049

When the curve is regular at x_0, we will trace this path to a substantial length by a path following scheme we propose. If this attempt fails, no such solution path may exist and x_0 will be classified as an isolated solution of $P(x) = 0$ with a multiplicity greater than one. When $P_X(x_0)$ has $k > 1$ very small singular values, we augment $P(x) = 0$ with $k-1$ generic hyperplanes $a_i^H(x - x_0) = 0$, $i = 1, \ldots, k-1$ at x_0. If the solution component $\mathcal{M}$ of $P(x) = 0$ in which x_0 lies is of dimension k, then the system

$$\bar{P}(x) = \begin{cases} P(x) = 0, \\ a_1^H(x - x_0) = 0, \\ \vdots \\ a_{k-1}^H(x - x_0) = 0 \end{cases} \tag{1.1}$$

will contain a one-dimensional solution component $\bar{\mathcal{M}}$ of $\bar{P}(x) = 0$ through x_0. When $\bar{\mathcal{M}}$ is regular at x_0, the assertion $\dim(\mathcal{M}) = k$ is accurate only if we can identify $\bar{\mathcal{M}}$ by tracing $\bar{\mathcal{M}}$ to a satisfactory length. If this path following cannot be carried out successfully, such a component $\bar{\mathcal{M}}$ may not exist. We will then remove hyperplane $a_{k-1}^H(x - x_0) = 0$ in (1.1) and restart our effort to identify the possible one-dimensional solution component $\bar{\bar{\mathcal{M}}}$ produced by the system

$$\bar{\bar{P}}(x) = \begin{cases} P(x) = 0, \\ a_1^H(x - x_0) = 0, \\ \vdots \\ a_{k-2}^H(x - x_0) = 0. \end{cases} \tag{1.2}$$

The existence of such one-dimensional component $\bar{\bar{\mathcal{M}}}$ implies the solution component $\mathcal{M}$ of $P(x) = 0$ is of dimension $k-1$. The process may be continued in the same manner when the failure repeats in identifying $\bar{\bar{\mathcal{M}}}$, and the dimension of $\mathcal{M}$ will ultimately (very soon in practice) be determined. We will elaborate the details in Section 3.

Our algorithm, listed in Section 3, has been successfully implemented (a Matlab module is available at: http://math.nuk.edu.tw/eng/02-02_people013.asp) and applied to a vast variety of polynomial systems. Generically, it may not be easy to assign a uniform threshold in determining the meaning of *smallness* of a singular value. In our algorithm, however, the choice of the magnitude of the threshold can safely be relaxed with no risk of possible mistakes. While the proposed algorithm is experimental, it has been tested successfully on the class of problems with the solution in question belonging to a reduced component. Numerical results exhibited in Section 4 illustrate the remarkable accuracy of our algorithm in determining the dimension of the solution component that contains a given solution x_0.

Our algorithm is particularly valuable when the homotopy continuation method is used to solve polynomial systems numerically which follows homotopy paths emanating from solutions of a known system to reach solutions of the target system at the end of those paths. It was widely believed that it is nongeneric for the repeated appearances of the same solution that lies on a positive dimensional solution component. Consequently, a solution that repeats itself at the end of different paths will always be taken as an isolated solution with a positive multiplicity if no apparent *curve jumping* exists. In contrary, this sort of repeated appearances of the same solution actually happens frequently in positive dimensional solution components from the results of our algorithm. For a simple example, the cyclic-4 problem [8, Example 2 in §4] has no isolated solutions. But, all 16 homotopy paths converge to 8 particular solutions repeatedly, twice for each one, regardless of what starting systems were used. Remarkably, our algorithm accurately determined the correct dimensions of the solution component on each individual case of this system.

Very recently, a subject called *numerical algebraic geometry* is proposed in a series of papers [9,10,12–14] (summarized in [11]), and a great progress has been achieved. In these articles, *witness sets* are the central concept and play a critical role of classifying irreducible solution components of polynomial systems of different dimensions. To accurately identify those witness sets relies on accurate determination of whether a computed zero of a polynomial system is isolated. For this purpose, we believe our algorithm presented in this paper, when it is fully developed, can substantially improve the efficiency and reliability of the algorithm currently employed in their method.

2. Preliminary

An inevitable part of our method to determine the dimension of a solution component is the rank revealing of the Jacobian matrix $P_X(x_0)$ at the solution x_0. This can normally be achieved by computing the SVD (Singular Value Decomposition) of $P_X(x_0)$ and deciding which singular values are significantly nonzero. However, in our context the rank deficiency of $P_X(x_0)$ is usually small compared to its size. It seems needless to compute the whole set of singular values to determine its rank. We therefore adopt in our algorithm the rank revealing technique recently developed in [6] which computes singular values and their associate singular vectors in ascending order from the smallest one. By which, we need only compute those singular values which are smaller than the given threshold to determine the rank of $P_X(x_0)$. The algorithm is briefly summarized below.

Let A be an $m \times n$ ($m \geqslant n$) matrix with complex entries, and let

$$\sigma_1 \leqslant \sigma_2 \leqslant \cdots \leqslant \sigma_n$$

be its singular values. Since the smallest singular value $\sigma_{\min} \equiv \sigma_1$ satisfies

$$\sigma_{\min} = \min_{\|y\|_2=1} \|Ay\|_2, \quad y \in \mathbb{C}^n,$$

the problem of finding $\sigma_{\min}$ can be converted to solving the overdetermined system

$$\begin{bmatrix} \rho y^H \\ A \end{bmatrix} y = \begin{bmatrix} \rho \\ 0 \end{bmatrix}, \tag{2.3}$$

where $\rho > \sigma_1$ and $[\cdot]^H$ is the conjugate transpose of $[\cdot]$. And this overdetermined system can be solved by using the Gauss–Newton iteration [2]

$$\begin{cases} y_{k+1} = y_k - \begin{bmatrix} 2\rho y_k^H \\ A \end{bmatrix}^{\dagger} \left[\begin{bmatrix} \rho y_k^H \\ A \end{bmatrix} y_k - \begin{bmatrix} \rho \\ 0 \end{bmatrix} \right], \\ \zeta_{k+1} = \dfrac{\|Ay_{k+1}\|_2}{\|y_{k+1}\|_2}, \quad k = 0, 1, \ldots. \end{cases} \tag{2.4}$$

Here, for a matrix B, $B^{\dagger}$ stands for its Moore–Penrose generalized inverse. Usually, the initial iterate y_0 is taken to be the solution of the least squares problem

$$\begin{bmatrix} \rho a^H \\ A \end{bmatrix} y_0 = \begin{bmatrix} \rho \\ 0 \end{bmatrix}, \tag{2.5}$$

where $a \in \mathbb{C}^n$ is a randomly chosen unit vector. This choice is based on the observation that when $a^H y \neq 0$ for $Ay = 0$ and the smallest singular value $\sigma_{\min}$ of A is zero, then the solution of (2.5) is the associated singular vector of A. Here and after, *singular vector* of A always represents the right singular vector of A when no ambiguities exist. It can be shown [6] that the Gauss–Newton iteration applied to (2.3) in (2.4) is essentially the application of the inverse iteration to the matrix $A^H A$. The global convergence of the iteration in (2.4) is therefore warranted, and (ζ_k, y_k) will converge to the singular pair (σ_1, v_1). Most importantly, after $\sigma_1 = \sigma_{\min}$ is calculated along with its associated singular vector v_1, this singular pair can be *deflated* by considering the matrix

$$A_\tau = \begin{bmatrix} \tau v_1^H \\ A \end{bmatrix}, \quad \tau \in \mathbb{R}.$$

This matrix has the same set of singular values as well as their associated singular vectors as those of A except the smallest singular value σ_1 of A is replaced by $\sqrt{\tau^2 + \sigma_1^2}$ in A_τ with associated singular vector v_1 [6]. So, if we choose $\tau = \|A\|_F$, then the replacement $\sqrt{\tau^2 + \sigma_1^2}$ becomes the largest singular value of A_τ. In the meantime, the second smallest singular value σ_2 of A becomes the smallest one of A_τ, and the iteration scheme for finding smallest singular pair given above can be applied to A_τ to calculate the singular pair (σ_2, v_2) of A. This process can be continued recursively to calculate as many singular values of A in ascending order as desired.

Summarizing the discussion above results in the following

Algorithm 1.

Input: $m \times n$ matrix A ($m \geqslant n$), tolerance $\bar{\sigma} > 0$.
Output: Singular values of A which are less than $\bar{\sigma}$ along with their associated singular vectors.

$S := \emptyset$, $V := \emptyset$.

Step 1. Find y_0 by solving linear least squares problem

$$\begin{bmatrix} \rho a^H \\ A \end{bmatrix} y_0 = \begin{bmatrix} \rho \\ 0 \end{bmatrix},$$

where $a \in \mathbb{C}^n$ is randomly chosen with $\|a\|_2 = 1$ and $\rho > \|A\|_F$.

Step 2. Solve overdetermined system

$$\begin{bmatrix} \rho y^H \\ A \end{bmatrix} y = \begin{bmatrix} \rho \\ 0 \end{bmatrix}$$

by the Gauss–Newton iteration

$$\begin{cases} y_{k+1} = y_k - \begin{bmatrix} 2\rho y_k^H \\ A \end{bmatrix}^{\dagger} \left[\begin{bmatrix} \rho y_k^H \\ A \end{bmatrix} y_k - \begin{bmatrix} \rho \\ 0 \end{bmatrix} \right], \\ \zeta_{k+1} = \dfrac{\|A y_{k+1}\|_2}{\|y_{k+1}\|_2}, \quad k = 0, 1, \ldots. \end{cases}$$

Let $\zeta_k \to \sigma$ and $y_k \to v$ as $k \to \infty$. If $\sigma > \bar{\sigma}$, stop. Otherwise,

$$S := S \cup \{\sigma\},$$
$$V := V \cup \{v\},$$
$$A := \begin{bmatrix} \tau v^H \\ A \end{bmatrix} \quad \text{with } \tau = \|A\|_F.$$

Go to step 1.

3. The method

Our method is essentially based on the fact [10] that if a generic point x_0 lies on a k-dimensional ($k \geqslant 2$) irreducible component $\mathcal{M}$ of the solution set of the polynomial equation $P(x) = (p_1(x), \ldots, p_n(x)) = 0$, where $x = (x_1, \ldots, x_n) \in \mathbb{C}^n$, then the intersection of $\mathcal{M}$ with a generic affine linear subspace L_{k-1} of dimension $n - (k-1)$ containing x_0 forms a one-dimensional solution set that passes through x_0. More precisely, write a generic linear subspace L_{k-1} of dimension $n - (k-1)$ that contains x_0 as

$$\begin{aligned} &a_1^H (x - x_0) = 0, \\ &\vdots \\ &a_{k-1}^H (x - x_0) = 0 \end{aligned}$$

with $a_i \in \mathbb{C}^n$ for $i = 1, \ldots, k-1$ being generically chosen. Then, there exists a one-dimensional solution set $\bar{\mathcal{M}}$ of

$$\bar{P}(x) = \begin{cases} P(x) = 0, \\ a_1^H (x - x_0) = 0, \\ \vdots \\ a_{k-1}^H (x - x_0) = 0 \end{cases} \tag{3.6}$$

that contains x_0. Accordingly, successful identification of such one-dimensional solution path of $\bar{P}(x) = 0$ ensures that x_0 lies on a k-dimensional solution component of $P(x) = 0$.

When a numerical solution x_0 of $P(x) = 0$ is obtained, we first calculate the set of singular values of $P_X(x_0)$ that are smaller than a given threshold $\bar{\sigma} > 0$ by Algorithm 1 in the last section. Since the absolute magnitude of a singular value σ of $P_X(x_0)$ can easily be manipulated by scaling the polynomial equations, only the relative magnitude of σ with respect to $\|P_X(x_0)\|_2$ plays the essential role here. While $\bar{\sigma} = 10^{-5}\|P_X(x_0)\|_2$ is used as a threshold in our program with no failures, bigger choices of $\bar{\sigma} > 0$ will cause no risks as explained later. If the set of singular values smaller than $\bar{\sigma} > 0$ admits k elements, we will start to identify the one-dimensional solution path $\bar{\mathcal{M}}$ of $\bar{P}(x) = 0$ in (3.6) by assuming the solution component $\mathcal{M}$ of $P(x) = 0$ that contains x_0 is of dimensional k. Successfully identifying $\bar{\mathcal{M}}$ would confirm the dimension of $\mathcal{M}$ *is* k in a neighborhood of x_0. Otherwise, changing the assumption of the dimension of $\mathcal{M}$ to be $k-1$, we will repeat our effort to identify the possible one-dimensional solution path $\bar{\mathcal{M}}$ of $\bar{P}(x) = 0$ in (3.6) with k replaced by $k-1$.

We take $k = 1$ as our point of departure for the details of this process.

3.1. $k = 1$ *(only one singular value of* $P_X(x_0)$ *is less than threshold* $\bar{\sigma} > 0$*)*

Since $\|P_X(x_0)\|_2$ admits only one relatively small singular value, the dimension of the irreducible solution component $\mathcal{M}$ of $P(x) = 0$ that contains x_0 can be no bigger than one. We will begin by assuming $\dim(\mathcal{M}) = 1$ in a neighborhood of x_0. To numerically trace $\mathcal{M}$, we modify the usual prediction–correction scheme for following a continuation path [1] as follows:

(1) Prediction:

Since any curve $x(t)$ in $\mathcal{M}$ with $t \in \mathbb{R}$ satisfies $P(x(t)) = 0$, hence,

$$P_X\big(x(t)\big)\frac{dx}{dt} = 0.$$

Therefore, the zero vector of $P_X(x_0)$ is a proper choice of the direction of the prediction at x_0. Let u be the singular vector associated with the smallest singular value of $P_X(x_0)$ with $\|u\|_2 = 1$. This vector closely approximates a zero vector of $P_X(x_0)$ and is freely available when the smallest singular value of $P_X(x_0)$ is calculated by Algorithm 1 in the last section. For a proper step length $\delta > 0$, let

$$x_1 = x_0 + \delta u$$

be our prediction.

(2) Correction:

By assumption $\dim(\mathcal{M}) = 1$, thus the augmented system

$$\tilde{P}(x) = \begin{cases} P(x) = 0, \\ (x - x_1)^H u = 0 \end{cases} \tag{3.7}$$

will produce an isolated solution in the neighborhood if the chosen step length $\delta > 0$ is sufficiently small. So, to come back to $\mathcal{M}$ from x_1, we may solve the overdetermined system (3.7) by Gauss–Newton's iteration

$$x^{m+1} = x^m - \big[J\tilde{P}\big(x^m\big)\big]^{\dagger}\tilde{P}\big(x^m\big), \quad m = 0, 1, \ldots, \tag{3.8}$$

with $x^0 = x_1$. When the iteration fails to converge, the prediction will be repeated with $\delta \leftarrow \frac{\delta}{2}$ followed by the correction. If the failure of convergence persists for δ less than a preassigned tolerance $\bar{\delta} > 0$ (we use $\bar{\delta} = 10^{-6}\|x_0\|_2$ in our program), then such solution component $\mathcal{M}$ may not exist and x_0 will be identified as an isolated solution of $P(x) = 0$.

If (3.8) converges to x_1^* with $\|P(x_1^*)\| < \varepsilon$ for a preassigned tolerance $\varepsilon > 0$, x_1^* will be taken as a numerical solution of $P(x) = 0$, and the above prediction–correction procedure will be repeated at x_1^*.

Remark 3.1. We choose the preassigned tolerance $\varepsilon > 0$ in tracing $\mathcal{M}$ based on the following observations. When a numerical solution x_0 of $P(x) = 0$ is given with an ultimate residue $\|P(x_0)\|_2 < \varepsilon_0$, it is rather restrictive and unnecessary to post ε_0 as a uniform tolerance for the error of $\|P(x_i^*)\|_2$ in tracing $\mathcal{M}$. Let x^e and x^* be the exact and numerical solutions of (3.7) satisfying $\tilde{P}(x^e) = 0$ and $\|\tilde{P}(x^*)\|_2 < \varepsilon$. Of course, they also satisfy $P(x^e) = 0$ and $\|P(x^*)\|_2 < \varepsilon$. Now Taylor series expansion at x^e yields

$$P(x^*) = P(x^e) + P_X(x^e)(x^* - x^e) + O(\|x^* - x^e\|^2)$$
$$\approx P_X(x^*)(x^* - x^e) \tag{3.9}$$

when $x^* \approx x^e$. So,

$$\|P(x^*)\|_2 \approx \|P_X(x^*)(x^* - x^e)\|_2$$
$$\leqslant \|P_X(x^*)\|_2 \|x^* - x^e\|_2. \tag{3.10}$$

When Gauss–Newton's iteration (3.8) converges to the numerical solution x^*, one usually stops the iteration when $\|x^* - x^e\|_2 \approx 10^{-16}\|x^*\|_2$ in double precision. Thus,

$$\|P(x^*)\|_2 \lessapprox 10^{-16}\|P_X(x^*)\|_2 \|x^*\|_2. \tag{3.11}$$

To allow $\|P(x_i^*)\|_2$ to grow within tolerance, we therefore choose

$$\varepsilon = \max\left\{l\varepsilon_0, 10^{-8} \times \sqrt{\|P_X(x_{i-1}^*)\|_2 \|x_{i-1}^*\|_2}\right\}$$

as our tolerance for the accuracy of $\|P(x_i^*)\|_2$. In our code, we set $l = 100$ to allow two more digits flexibility than the accuracy of $\|P(x_0)\|_2$ and it never fails in all our experiments.

The prediction–correction scheme discussed above can be continued consecutively to produce a sequence of points $x_1^*, x_2^*, \ldots$, along with successful step sizes $\delta_1, \delta_2, \ldots$. To terminate the path following with the assurance of the existence of solution path $\mathcal{M}$ that contains x_0, the accumulated successful step sizes must reach a substantial amount. From (3.7), it is clear that

$$\|x_i^* - x_{i-1}^*\|_2 \geqslant \delta_i, \quad i = 1, 2, \ldots,$$

thus,

$$\sum_{i=1}^{m} \|x_{i-1}^* - x_i^*\|_2 \geqslant \sum_{i=1}^{m} \delta_i \equiv s(m) \quad \text{for } m > 1.$$

We will admit the existence of $\mathcal{M}$ if $s(m)$ is bigger than a preassigned length $\eta > 0$ for certain $m > 1$. If the sum of successful step sizes can never reach η, x_0 will be classified as an isolated solution of $P(x) = 0$.

Remark 3.2. The preassigned length $\eta > 0$ should be chosen relative to the size of $\|x_0\|_2$. In our program, we use $\eta = 10^{-1}\|x_0\|_2$ if $\|x_0\|_2 > 5$, $\eta = 0.5$ otherwise.

3.2. $k \geqslant 2$ ($P_X(x_0)$ has more then one singular values less than threshold $\bar{\sigma} > 0$)

When $k \geqslant 2$, the maximal possible dimension of the solution component $\mathcal{M}$ of $P(x) = 0$ in a neighborhood of x_0 is k. Therefore we assume $\dim(\mathcal{M}) = k$ in a neighborhood of x_0 in the beginning. Let $\sigma_1, \ldots, \sigma_k$ be those singular values of $P_X(x_0)$ which are less than the tolerance $\bar{\sigma} > 0$ and $v_1, \ldots, v_k$ be the corresponding orthonormal singular vectors, respectively. With $k - 1$ generic hyperplanes

$$a_i^H(x - x_0) = 0, \quad i = 1, \ldots, k - 1,$$

where $a_i \in \mathbb{C}^n$ are generically chosen, consider the system

$$\bar{P}(x) = \begin{cases} P(x) = 0, \\ a_1^H(x - x_0) = 0, \\ \vdots \\ a_{k-1}^H(x - x_0) = 0. \end{cases} \tag{3.12}$$

Since $\dim(\mathcal{M}) = k$, there is a one-dimensional solution path $\bar{\mathcal{M}}$ of $\bar{P}(x) = 0$ contained in $\mathcal{M}$ that contains x_0.

For any curve $\{x(t)\} \subset \bar{\mathcal{M}}$ with $t \in \mathbb{R}$ satisfying $\bar{P}(x(t)) = 0$, we have

$$\bar{P}_X\big(x(t)\big)\frac{dx}{dt} = 0,$$

where

$$\bar{P}_X\big(x(t)\big) = \begin{bmatrix} P_X(x(t)) \\ a_1^H \\ \vdots \\ a_{k-1}^H \end{bmatrix}$$

is of rank $n-1$ since the numerical rank of $P_X(x(t))$ is taken to be $n-k$. Its kernel is therefore one-dimensional, and its zero vector is a suitable prediction direction at $x(t)$. To begin the path following scheme to trace $\bar{\mathcal{M}}$ at x_0 as described in Section 3.1, the already computed singular vectors $v_1, \ldots, v_k$ of $P_X(x_0)$ expand the kernel of $P_X(x_0)$ and the $(k-1) \times k$ matrix

$$A \equiv \begin{bmatrix} a_1^H \\ \vdots \\ a_{k-1}^H \end{bmatrix} [v_1, \ldots, v_k]$$

is of rank $k-1$. So if $Ac = 0$ for $c = (c_1, \ldots, c_k)^\top \in \mathbb{C}^k$, then

$$u \equiv [v_1, \ldots, v_k] \begin{bmatrix} c_1 \\ \vdots \\ c_k \end{bmatrix} \tag{3.13}$$

is a zero vector of $\bar{P}_X(x_0)$. In the process of tracing the one-dimensional solution path $\bar{\mathcal{M}}$ at a numerical solution x_i^* of $\bar{P}(x) = 0$ by using the prediction–correction scheme, we calculate a unit singular vector u of $\bar{P}_X(x_i^*)$ corresponding to its smallest singular value that is less than $\bar{\sigma} > 0$ and use u (with a proper sign) as the prediction direction at x_i^*. Since the numerical rank of $\bar{P}_X(x_i^*)$ is $n-1$, it must have a very small singular value. If no such singular value exists, the path following attempt will be restarted from x_0 by reconsidering the system $\bar{P}(x) = 0$ in (3.12) with k replaced by $k-1$. On the other hand, if the path tracing succeeds in continuation but fails to reach the preassigned satisfactory total length ultimately, path following will also be restarted at x_0 by replacing k by $k-1$ in (3.12).

When k is replaced by $k-1$ in (3.12), $\bar{P}_X(x_0)$ becomes rank-2 deficient numerically. Applying Algorithm 1 in the last section will produce two singular values $\bar{\sigma}_1 < \bar{\sigma}_2$ of $\bar{P}_X(x_0)$ that are less than $\bar{\sigma} > 0$ along with their associated singular vectors $\bar{v}_1$ and $\bar{v}_2$. In theory, both $\bar{\sigma}_1$ and $\bar{\sigma}_2$ are equal to zero *exactly*, and thus any direction in the linear span of $\bar{v}_1$ and $\bar{v}_2$ can be used as our prediction direction at x_0 to trace $\bar{\mathcal{M}}$. In practice, however, while both $\bar{\sigma}_1$ and $\bar{\sigma}_2$ are less than $\bar{\sigma} > 0$, there usually exists a (relatively) big gap between them, for instance, $\bar{\sigma}_1 = 10^{-12}$ and $\bar{\sigma}_2 = 10^{-5}$. Apparently, in such situations, the direction of singular vector $\bar{v}_1$ is much closer to the tangent direction of $\bar{\mathcal{M}}$. Therefore, we first use $\bar{v}_1$ as our prediction direction at x_0. In the process of tracing $\bar{\mathcal{M}}$, however, $\bar{P}_X(x_i^*)$ remains rank-1 deficient generically at numerical solution x_i^* of $\bar{P}(x) = 0$ for $i > 0$, and the singular vector u associated with the smallest singular value of $\bar{P}_X(x_i^*)$ can be used as the prediction direction at x_i^*. If this path tracing fails, we will use $\bar{v}_2$ as our prediction direction at x_0 in our next attempt. In general, the assumption of the dimension of $\mathcal{M}$ will further be reduced only when we exhaust using all singular vectors associated with those singular values of $\bar{P}_X(x_0)$ that are less than $\bar{\sigma} > 0$ as the prediction direction at x_0.

In the procedure described above, apparently there is no risk to relax the choice of the magnitude of $\bar{\sigma} > 0$ as a threshold to decide which singular values should be accounted for zero singular values practically. While extra singular values may join the set when the threshold $\bar{\sigma} > 0$ becomes bigger, this will not affect our algorithm in determining the accurate dimensionality of the solution component. Of course, the amount of extra computations can be limited if the threshold $\bar{\sigma} > 0$ is chosen to be *reasonably* small.

The details of our algorithm to determine the dimension of the solution component $\mathcal{M}$ of $P(x) = 0$ in which x_0 lies is given below.

Algorithm 2.

Input: Polynomial equations $P(x) = (p_1(x), \ldots, p_n(x))$.
Numerical solution x_0 of $P(x) = 0$ along with $P_X(x_0)$.
Tolerance parameters: $\bar{\sigma} > 0$, $\bar{\delta} > 0$, $\eta > 0$.
Output: Dimension of the solution component of $P(x) = 0$ that contains x_0.

Step 0. By Algorithm 1, find all singular values $\sigma_1 \leqslant \cdots \leqslant \sigma_{k_0}$ of $P_X(x_0)$ which are less than $\bar{\sigma}$ along with their associated singular vectors $v_1, v_2, \ldots, v_{k_0}$. Set $V_0 := \{v_1, \ldots, v_{k_0}\}$, $x_0^* := x_0$.
If $k_0 = 0$, then print "x_0 is an isolated solution" and stop.
Otherwise, set $S(0) = 0$, $\delta_0 = 0.5 \times \eta$.
If $k_0 = 1$, set $\bar{P}(x) := P(x)$, $\bar{v}_1 := v_1$, $j := 1$, $\bar{k} := 1$. Go to step 1.2.
Otherwise, generate $k_0 - 1$ random vectors $a_1, \ldots, a_{k_0-1}$ in $\mathbb{C}^n$ with their sizes being similar to $\|P_X(x_0)\|$.
Set

$$\bar{P}(x) := \begin{cases} P(x), \\ a_1^H(x - x_0), \\ \vdots \\ a_{k_0-1}^H(x - x_0), \end{cases}$$

$k := k_0$, $j := 1$, $\bar{k} := 1$. Go to step 1.1.

Step 1.

Step 1.1. Find unit vector

$$u := \sum_{i=1}^{k} c_i v_i$$

in the kernel of $n \times (k-1)$ matrix $[a_1, \ldots, a_{k-1}]$, where $v_i \in V_0$ and $c_i \in \mathbb{C}$ for $i = 1, \ldots, k$. Set $\bar{x} := x_0 + \delta_0 u$, $i := 0$. Go to step 2.
Step 1.2. Set $u := \bar{v}_j$, $\bar{x} := x_0 + \delta_0 u$, $i := 0$. Go to step 2.

Step 2.

Step 2.1. Set $\tilde{P}(x) := \begin{cases} \bar{P}(x), \\ u^H(x - \bar{x}). \end{cases}$
Step 2.2. Solve $\tilde{P}(x) = 0$ by Gauss–Newton's iteration

$$x^{m+1} = x^m - \left[J\tilde{P}\left(x^m\right)\right]^{\dagger} \tilde{P}\left(x^m\right), \quad m = 0, 1, \ldots,$$

with $x^0 = \bar{x}$.
If it converges, set $x_{i+1}^* :=$ the limit, $\delta_{i+1} := \min\{2\delta_i, \delta_0\}$, and $S(i+1) := S(i) + \delta_i$.
If $S(i+1)$ or $\|x_{i+1}^* - x_0\|$ is bigger than η, then print "Dimension of the solution component that contains x_0 is k" and stop.
Otherwise, go to step 3.
Otherwise, $\delta_i := \frac{\delta_i}{2}$.
If $\delta_i < \bar{\delta}$, go to step 4.
Otherwise, $\bar{x} = x_i^* + \delta_i u$. Go to step 2.1.

Step 3. Calculate smallest singular value $\bar{\sigma}_1$ of $\bar{P}_X(x_{i+1}^*)$ and its associated singular vector v by Algorithm 1.
If $\bar{\sigma}_1 > \bar{\sigma}$, go to step 4.
Otherwise, choose a proper sign of v which forms a smaller angle with $x_{i-1}^* - x_i^*$. Set $u := v$, $\bar{x} := x_{i+1}^* + \delta_{i+1} u$ and $i := i + 1$. Go to step 2.

Step 4. Set $j := j + 1$.
If $j \leqslant \bar{k}$, go to step 1.2.
Otherwise, set $k := k - 1$, $j := 1$.
If $k \geqslant 2$, go to step 4.1.
If $k = 1$, go to step 4.2.
If $k = 0$, print "x_0 is an isolated solution" and stop.

Step 4.1. Set $\bar{P}(x) := \begin{cases} P(x), \\ a_1^H(x - x_0), \\ \vdots \\ a_{k-1}^H(x - x_0). \end{cases}$
By Algorithm 1, find all singular vectors $\bar{V} := \{\bar{v}_1, \ldots, \bar{v}_l\}$ of $\bar{P}_X(x_0)$ corresponding to its singular values that are less than $\bar{\sigma}$. Set $\bar{k} := l$. Go to step 1.2.

Step 4.2. Set $\bar{P}(x) := P(x)$, $\bar{k} := k_0$, $\bar{V} := \{\bar{v}_1, \ldots, \bar{v}_{\bar{k}}\}$, where $\bar{v}_i = v_i$, $v_i \in V_0$ for $i = 1, \ldots, \bar{k}$. Go to step 1.2.

4. Numerical results

Our algorithm for determining the dimension of the solution component that contains a given numerical solution x_0 of a polynomial system $P(x) = 0$ has been successfully implemented in Matlab and C++. It has been tested on a large variety of known polynomial systems and the results are constantly accurate. While the numerical solutions of the polynomial systems in the examples listed below were all provided by the homotopy continuation method, our algorithm is equally applicable to numerical solutions of the systems by any other methods.

Example 1. For $(x_1, x_2, x_3) \in \mathbb{C}^3$, consider the polynomial system [12]:

$$p_1(x_1, x_2, x_3) = \big(x_2 - x_1^2\big)\big(x_1^2 + x_2^2 + x_3^2 - 1\big)(x_1 - 0.5),$$
$$p_2(x_1, x_2, x_3) = \big(x_3 - x_1^3\big)\big(x_1^2 + x_2^2 + x_3^2 - 1\big)(x_2 - 0.5),$$
$$p_3(x_1, x_2, x_3) = \big(x_2 - x_1^2\big)\big(x_3 - x_1^3\big)\big(x_1^2 + x_2^2 + x_3^2 - 1\big)(x_3 - 0.5).$$

Obviously, the solution set of this system consists of

1. A two-dimensional component $x_1^2 + x_2^2 + x_3^2 = 1$.
2. Four one-dimensional components
   (a) line $x_1 = 0.5$, $x_3 = (0.5)^3$,
   (b) line $x_1 = \sqrt{0.5}$, $x_2 = 0.5$,
   (c) line $x_1 = -\sqrt{0.5}$, $x_2 = 0.5$,
   (d) twisted cubic $x_2 = x_1^2$, $x_3 = x_1^3$.
3. One isolated solution $x_1 = 0.5$, $x_2 = 0.5$, $x_3 = 0.5$.

When the polyhedral homotopy continuation method was used to solve the system, 129 numerical solutions were obtained. Our algorithm is applied to all those solutions and the result shows:

- 112 of them lie on 2-dimensional component,
- 16 of them lie on 1-dimensional components (4 on line 2(a), 4 on line 2(b), 4 on line 2(c), 4 on line 2(d)),
- 1 isolated solution.

Example 2. The *cyclic-4* polynomial system [8]:

$$p_1(x_1, x_2, x_3, x_4) = x_1 + x_2 + x_3 + x_4,$$
$$p_2(x_1, x_2, x_3, x_4) = x_1x_2 + x_2x_3 + x_3x_4 + x_1x_4,$$

$$p_3(x_1, x_2, x_3, x_4) = x_1x_2x_3 + x_2x_3x_4 + x_1x_3x_4 + x_1x_2x_4,$$
$$p_4(x_1, x_2, x_3, x_4) = x_1x_2x_3x_4 - 1.$$

It is known that the solution set of this system consists of two 1-dimensional components:

1. $\{(x_1, x_2, x_3, x_4) \in \mathbb{C}^4 \mid x_1 + x_3 = 0,\ x_2 + x_4 = 0,\ x_1x_2 = 1\}$,
2. $\{(x_1, x_2, x_3, x_4) \in \mathbb{C}^4 \mid x_1 + x_3 = 0,\ x_2 + x_4 = 0,\ x_1x_2 = -1\}$.

The polyhedral homotopy continuation method provides 16 numerical solutions. Those 16 homotopy paths always arrive at the same 8 solutions, twice at each one, regardless of what the starting systems were used. They are: for $i = \sqrt{-1}$,

- $(1, 1, -1, -1), (-1, -1, 1, 1), (i, -i, -i, i), (-i, i, i, -i) \in$ component 1,
- $(1, -1, -1, 1), (-1, 1, 1, -1), (i, i, -i, -i), (-i, -i, i, i) \in$ component 2.

Notice that none of those solutions are isolated. It was widely believed previously when the homotopy method is used, this sort of repeated appearances of the same solution was not permitted to occur on solution component of positive dimension generically. So, once the repetition occurs, the solution will always be identified as an isolated solution with multiple multiplicity if the *curve jumping* is declared absent. However, our algorithm accurately determined that the dimensions of the components to which those solutions belong individually are all equal to one. In fact, this phenomenon appears in many other systems we have tested, such as cyclic-8 and cyclic-9 systems [8], and our algorithm never fails in any one of those cases.

One can show by hand that Jacobians at those solutions all have two zero singular values, they are all rank-2 deficient. In our numerical result, all of the minimal singular values $\sigma_{\min}$ of the Jacobian matrices at those 16 solutions are bigger than $10^{-13}\|P_X(x_0)\|_2$. We can see that choosing $\bar{\sigma} = 10^{-13}\|P_X(x_0)\|_2$ or smaller as our threshold will result in numerical inaccuracy since 8 of them will mistakenly be judged as isolated solutions.

Example 3. The *Caprasse* polynomial system [8]:

$$p_1(x_1, x_2, x_3, x_4) = x_2^2x_3 + 2x_1x_2x_4 - 2x_1 - x_3,$$
$$p_2(x_1, x_2, x_3, x_4) = 4x_1x_2^2x_3 - x_1^3x_3 + 4x_1^2x_2x_4 + 2x_2^3x_4 + 4x_1^2 - 10x_2^2 + 4x_1x_3 - 10x_2x_4 + 2,$$
$$p_3(x_1, x_2, x_3, x_4) = 2x_2x_3x_4 + x_1x_4^2 - x_1 - 2x_3,$$
$$p_4(x_1, x_2, x_3, x_4) = 4x_2x_3^2x_4 - x_1x_3^3 + 4x_1x_3x_4^2 + 2x_2x_4^3 + 4x_3^2 - 10x_4^2 + 2.$$

The solution set of this system is known to have

$\mathbb{S}_1$: 8 isolated solutions with multiplicity 4 of each,
$\mathbb{S}_2$: 24 nonsingular isolated solutions.

Applying polyhedral homotopy continuation method to this system yields 56 numerical solutions. For our choice $\bar{\sigma} = 10^{-5}\|P_X(x_0)\|_2$, 24 solutions in $\mathbb{S}_2$ are automatically classified as nonsingular isolated solutions. All the rest of the solutions in $\mathbb{S}_1$ were also determined to be isolated since our algorithm could not identify any positive dimensional solution component that contains any one of them. Checking back the homotopy paths, actually 8 of those 32 solutions were all reached by 4 homotopy paths with different slopes. Apparently the *curve jumping* is absent, and those 8 solutions were all isolated solutions of multiplicity 4 indeed.

Example 4. The *Cassou–Nogus* polynomial system [8]: for $x = (x_1, x_2, x_3, x_4) \in \mathbb{C}^4$,

$$p_1(x) = 15x_1^4x_2x_3^2 + 6x_1^4x_2^3 + 21x_1^4x_2^2x_3 - 144x_1^2x_2 - 8x_1^2x_2^2x_4 - 28x_1^2x_3x_3x_4 - 648x_1^2,$$
$$p_2(x) = 30x_1^4x_2^3x_3 - 32x_2x_3x_4^2 - 720x_1^2x_2x_3 - 24x_1^2x_2^3x_4 - 432x_1^2x_2^2 + 576x_2x_4$$
$$- 576x_3x_4 + 16x_1^2x_2x_3^2x_4 + 16x_3^2x_4^2 + 16x_2^2x_4^2 + 9x_1^4x_2^4 + 39x_1^4x_2^2x_3^2$$

Table 1

	♯ of solutions $x \in \mathbb{S}$ with $\sigma_{\min}(P_X(x)) < \bar{\sigma}$
$\bar{\sigma} = 10^{-5}\|P_X(x)\|_2$	14
$\bar{\sigma} = 10^{-7}\|P_X(x)\|_2$	8
$\bar{\sigma} = 10^{-9}\|P_X(x)\|_2$	6
$\bar{\sigma} = 10^{-13}\|P_X(x)\|_2$	6
$\bar{\sigma} = 10^{-15}\|P_X(x)\|_2$	0

$$
\begin{aligned}
&+ 18x_1^4x_2x_3^3 - 432x_1^2x_3^2 + 24x_1^2x_3^3x_4 - 16x_1^2x_2^2x_3x_4 - 240x_2 + 5184,\\
p_3(x) &= 216x_1^2x_2x_3 - 162x_1^2x_3^2 - 81x_1^2x_2^2 + 1008x_2x_4 - 1008x_3x_4 - 15x_1^2x_2^3x_4\\
&+ 15x_1^2x_2^2x_3x_4 - 80x_2x_3x_4^2 + 40x_3^2x_4^2 + 40x_2^2x_4^2 + 5184,\\
p_4(x) &= 4x_1^2x_2x_3 - 3x_1^2x_3^2 - 4x_1^2x_2^2 + 22x_2x_4 - 22x_3x_4 + 261.
\end{aligned}
$$

It is known that the solution set $\mathbb{S}$ of this system contains 16 nonsingular isolated solutions, and when the polyhedral homotopy continuation method was used we reached 16 numerical solutions. When our algorithm was applied with threshold $\bar{\sigma} = 10^{-5}\|P_X(x_0)\|_2$, all 16 solutions were classified as isolated solutions even though their Jacobians may have many singular values that are smaller than $\bar{\sigma}$.

Table 1 gives distribution of minimal singular values $\sigma_{\min}$ of the Jacobian matrix with different thresholds at those 16 solutions.

From Table 1 we can see that without our algorithm one must choose the threshold $\bar{\sigma}$ to be $10^{-15}\|P_X(x_0)\|_2$ or less to correctly determine the nonsingularity of all those 16 isolated solutions. But if we assign the threshold $\bar{\sigma} = 10^{-15}\|P_X(x_0)\|_2$, then all 16 numerical solutions in cyclic-4 problem in Example 2 will all be wrongfully determined as nonsingular isolated solutions. In fact, our algorithm was originally motivated by the difficulty of deciding a uniform threshold in determining the isolated solutions shown by those examples.

Example 5. For $(x_1, x_2, x_3) \in \mathbb{C}^3$, consider the polynomial system:

$$
\begin{aligned}
p_1(x_1, x_2, x_3) &= \left(x_2 - x_1^2\right)^2(x_1 + x_2 - 1),\\
p_2(x_1, x_2, x_3) &= \left(x_2 - x_1^2\right)^2(x_2 + x_3 - 1),\\
p_3(x_1, x_2, x_3) &= \left(x_2 - x_1^2\right)^2(x_1 + x_3 - 1).
\end{aligned}
$$

Obviously, the solution set of this system consists of

1. A one-dimensional *nonreduced* component $x_2 = x_1^2$.
2. One isolated solution $x_1 = 0.5$, $x_2 = 0.5$, $x_3 = 0.5$.

We use this example to demonstrate that our algorithm may sometimes be successful when applied to the solution component that contains a given solution x_0 is *nonreduced*. When one intends to follow a one-dimensional nonreduced solution component $\mathcal{M}$, Eq. (3.7) will produce an isolated solution with multiple multiplicity. The occurrence of such situations can be detected by the losing of the superlinear convergence of the Gauss–Newton iteration (3.8). On the other hand, the dismal barrier of attainable accuracy which may barricade the path following to reach the preassigned tolerance $\epsilon > 0$ as described in Remark 3.1 can be overcome by the deflation technique recently developed in [7].

When the polyhedral homotopy continuation method was used to solve the above system, 28 numerical solutions were obtained. Our algorithm is applied to all those solutions and the result shows:

- 27 of them lie on the 1-dimensional nonreduced component.
- 1 isolated solution.

In our algorithm, when the deflation method was employed in the Gauss–Newton iteration (3.8), all solutions $\bar{x} = (\bar{x}_1, \bar{x}_2, \bar{x}_3)$ lying on the 1-dimensional component $(x_2 = x_1^2)$ can all be followed within the preassigned tolerance as given in Remark 3.1.

References

[1] E.L. Allgower, K. Georg, Numerical path following, in: P.G. Ciarlet, J.L. Lions (Eds.), Handb. Numer. Anal., vol. 5, North-Holland, 1997, pp. 3–203.
[2] J.P. Dedieu, M. Shub, Newton's method for over-determined system of equations, Math. Comp. 69 (1999) 1099–1115.
[3] T.Y. Li, Numerical solution of multivariate polynomial systems by homotopy continuation methods, Acta Numer. 6 (1997) 399–436.
[4] T.Y. Li, Solving polynomial systems by polyhedral homotopies, Taiwanese J. Math. 3 (3) (1999) 251–279.
[5] T.Y. Li, Numerical solution of polynomial systems by homotopy continuation methods, in: F. Cucker (Ed.), Handb. Numer. Anal., vol. 11, North-Holland, 2003, pp. 209–304.
[6] T.Y. Li, Z. Zeng, A rank-revealing method with updating, downdating and applications, SIAM J. Matrix Anal. Appl. 26 (4) (2005) 918–946.
[7] A. Leykin, J. Verschelde, A. Zhao, Newton's method with deflation for isolated singularities of polynomial systems, Theoret. Comput. Sci. 359 (1–3) (2006) 111–122.
[8] B. Mourrain, The handbook of polynomial systems, available at http://www.inria.fr/safir/POL/index.html.
[9] A.J. Sommese, J. Verschelde, Numerical homotopies to compute generic points on positive dimensional algebraic sets, J. Complexity 16 (3) (2000) 572–602.
[10] A.J. Sommese, C.W. Wampler, Numerical algebraic geometry, in: J. Renegar, M. Shub, S. Smale (Eds.), The Mathematics of Numerical Analysis, Proceedings of the 1995 AMS–SIAM Summer Seminar in Applied Mathematics, Park City, Utah, in: Lectures in Appl. Math., vol. 32, 1996, pp. 749–763.
[11] A.J. Sommese, C.W. Wampler, The Numerical Solution of Systems of Polynomials, World Scientific Publishing Co., Singapore, 2005.
[12] A.J. Sommese, J. Verschelde, C.W. Wampler, Numerical decomposition of the solution sets of polynomial systems into irreducible components, SIAM J. Numer. Anal. 38 (6) (2001) 2022–2046.
[13] A.J. Sommese, J. Verschelde, C.W. Wampler, Using monodromy to decompose solution sets of polynomial systems into irreducible components, in: C. Ciliberto, F. Hirzebruch, R. Miranda, M. Teicher (Eds.), Application of Algebraic Geometry to Coding Theory, Physics and Computation, Proceedings of a NATO Conference, February 25–March 1, 2001, Eilat, Israel, Kluwer Academic Publishers, 2001, pp. 297–315.
[14] A.J. Sommese, J. Verschelde, C.W. Wampler, Symmetric functions applied to decomposing solution set of polynomial systems, SIAM J. Numer. Anal. 40 (6) (2002) 2026–2046.
[15] J. Verschelde, Algorithm 795: PHCpack a general-purpose solver for polynomial systems by homotopy continuation, ACM Trans. Math. Software 25 (2) (1999) 251–276.